V2 of the GMI Tropospheric CTM: Accomplishments since V1
by Bryan Duncan

The purposes of this document are to detail the major accomplishments since the release of the version 1 (V1) simulations in mid-October and to serve as a progress report.

We are happy to announce that we are currently preparing to run version 2 (V2) of the GMI Tropospheric CTM. This version will be used to write our first set of papers, including the initial model description paper. We will use the following meteorological fields: GISS II', DAO-STRAT, and GEOS-4 Atmospheric GCM (a.k.a. fvGCM). Due to a lack of information concerning convection, we will not include the MACCM3 meteorological fields in these manuscripts.

The activities described below are part of a continuing group effort, carried out by the GMI programmers (Jules Kouatchou, Bigyani Das, Maharaj Bhat, Steve Steenrod, and Hamid Oloso), Dan Bergmann, Jose Rodriguez, Susan Strahan, and Bryan Duncan, with input from the GMI science team members.

Some of the modifications that we report here, not only impact the Tropospheric version of the GMI model, but also the Combo version.

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Reminder of V1 Accomplishments
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1) The chemical mechanism was updated with recent experimental data, such as the removal of $O(^1D)$ by several atmospheric molecules [*Dunlea and Ravishankara*, 2004]. Absorption cross-sections for several species were also updated for use in Fast-J.

2) Many short-lived species in the stratosphere were given 1-day lifetimes to keep their concentrations from building there.

3) The species that are wet and/or dry deposited were updated to be the same as in GEOS-CHEM. This included adding several new species to be dry deposited: PMN, PPN, R4N2, and N_2O_5. A bug concerning HNO_3 dry deposition was corrected.

4) The transport of short-lived species like OH was "turned off".

5) A number of minor bugs were corrected.

6) The P-L diagnostic was modified to be 3-D, as opposed to 2-D (i.e., zonal average).

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Summary of V2 Accomplishments
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Our evaluation activities since the release of V1 included the comparison of model output with observations from field campaigns, satellites (i.e., TOMS, MOPITT, GOME), and surface sites. In addition, we participated in a model inter-comparison of the Intergovernmental Panel on Climate Change; our results fell in the "middle of the pack" as compared to the other participants, which is encouraging.

Here is a summary of our development activities for the GMI Tropospheric CTM since V1:

1) The GMI CTM now simulates the radiative and heterogeneous chemical effects of sulfate, dust, sea-salt, organic carbon and black carbon aerosol on tropospheric photochemistry. The 3-D aerosol mass distributions were calculated off-line using the Goddard Chemistry Aerosol Radiation and Transport (GOCART) model [*Chin et al.*, 2002]. The radiative and heterogeneous chemical effects of aerosols were implemented following *Martin et al.* [2003]. The net effect of aerosols on the tropospheric OH burden was small, but the changes for specific regions were quite dramatic.

1a) Heterogeneous Chemistry

Originally, the GMI Tropospheric CTM simulated only heterogeneous chemistry on sulfate aerosols.

The loss rate ($k_{het}=s^{-1}$) of trace gases on aerosol surfaces is calculated in the following way:

$$k_{het} = \sigma * [r /D_g + 4/(\nu \gamma)]^{-1}$$

where
r = radius of aerosol (cm)
σ = surface area of aerosols/volume of air (cm^2/cm^3)
D_g = gas phase diffusion coefficient (cm^2/s)
γ = probability of reaction per collision (unitless)
ν = mean molecular speed (cm/s) = $[8RT / (\pi * M_x)]^{0.5}$
R = universal gas constant
T = temperature (K)
M_x = molecular weight of trace gas, x

The term, r /D_g, accounts for the effect of gas-phase diffusion to the particle surface. This term was not included in the V1 formulation, which is appropriate in the low-pressure limit.

γ for N_2O_5 + aerosol is now a function of aerosol type, relative humidity, and temperature following the work of Mat Evans as implemented in GEOS-CHEM. The reaction probability is a constant value of 0.01 on dust aerosols, and 0.005 on black carbon. Expressions for the

reaction probability as a function of relative humidity for sulfate, organic carbon, and sea salt aerosols can be found at: http://www-as.harvard.edu/chemistry/trop/geos/geos_mech.html

The heterogeneous chemical modifications to the chemistry module required a significant modification to the chemical mechanism generator, KMG.

1b) Radiative Impacts: Now the aerosol optical depths are accounted for in Fast-J.

2) The stratospheric flux of the synthetic ozone tracer, Synoz, was increased from 475 Tg/yr to 550 Tg/yr to agree with present knowledge. In addition, we conducted a 25-yr spin-up of both Synoz and Nodoz, the synthetic nitrogen tracer, with the purpose to achieve steady-state. This change will impact any version of the code which estimates the tropopause height where Synoz = 150 ppbv. The tropopause height is now lower in altitude than before.

3) Entrainment/detrainment and downdraft code for convection was implemented to correct a known deficiency in the GMI Tropospheric model concerning the GISS meteorological fields. As a generalization, the impact of this new code was to increase boundary layer concentrations of many species and decrease them in the middle troposphere. Not surprisingly, the impact was greatest for short-lived and soluble species. The net impact on global tropospheric burdens appeared to be small though (e.g., $\Delta OH=0.95\%$, $\Delta O_3=1\%$, $\Delta NO_x=0.3\%$). This modification also impacts the Combo simulation.

4) A bug in the code that interpolated aircraft emissions was corrected. This bug resulted in annual emissions of nitrogen increasing from about 0.46 Tg N to about 0.57 Tg N. This correction will impact the Combo simulations as well.

5) Extra DAO-STRAT meteorological fields had been erroneously added to February, sometime in the distant past. This bug caused changes in monthly average CO and O_3 of +/- 5% in the troposphere. We first noticed the problem when trying to achieve steady-state with Synoz by doing a 25-year Synoz-only simulation. The Synoz stratospheric burden was oscillating +/- 5% with a period of 5-6 years. This correction will impact any version of the code using these meteorological fields.

6) Several minor bugs were flushed out during evaluation of model simulations.

7) MNO3 was removed from the constituent list as its source (i.e., PAN -> MNO3) was removed from the reaction list as suggested by Harvard. Attention: MNO3 was species #43, so any species with a higher number will be shifted back one. We will remove this species from the Combo chemical mechanism soon.

8) A number of new emissions diagnostics (for the Tropospheric and Combo versions) were added to aid scientific study:
   a) Surface emissions for species calculated on-line (i.e., N from soils, CO from monoterpene oxidation, CO from methanol oxidation, and propene from vegetation).
   b) 3-D information on total emissions for a given species from all sources.

9) A new parameterization for the calculation of the saturation vapor pressure over ice was implemented; the impact was minor.

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Work in Progress

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1) We will complete implementation of the lightning emissions parameterization, which is a function of the meteorological fields, from Dale Allen and Ken Pickering.

2) We obtained and are implementing several new meteorological fields to drive transport in the CTM:
   a) GEOS-4-DAS fields [Goddard Earth Observing System (GEOS) data assimilation systems (DAS), version 4] from the Goddard Modeling and Assimilation Office (GMAO)
   b) GEOS-4 DAS forecast fields (GEOS-4-Forecast),
   c) Oslo/European Centre DAS forecast fields (Oslo/EC-Forecast) from Oslo University and U. California, Irvine
   d) GEOS-4 Atmospheric GCM fields (GEOS-4-AGCM).

3) We are continuing comparison of model output to several satellite data sets, including GOME NO_2, TOMS ozone, and MOPITT CO.

4) Now that the aerosol code is in place, we are implementing it in the COMBO model as well. We will use the output from the GMI Aerosol model, in addition to the aerosols from the GOCART model, to simulate the impact of aerosols on trace gas photochemistry.

5) We will address shortly the issue of erroneous diffusion of aircraft emissions by vertical regridding, especially important for the COMBO model when doing studies of the UT/LS region.

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References

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